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RELAXATION AT CRITICAL POINTS: DETERMINISTIC AND STOCHASTIC THE--ETC(U)
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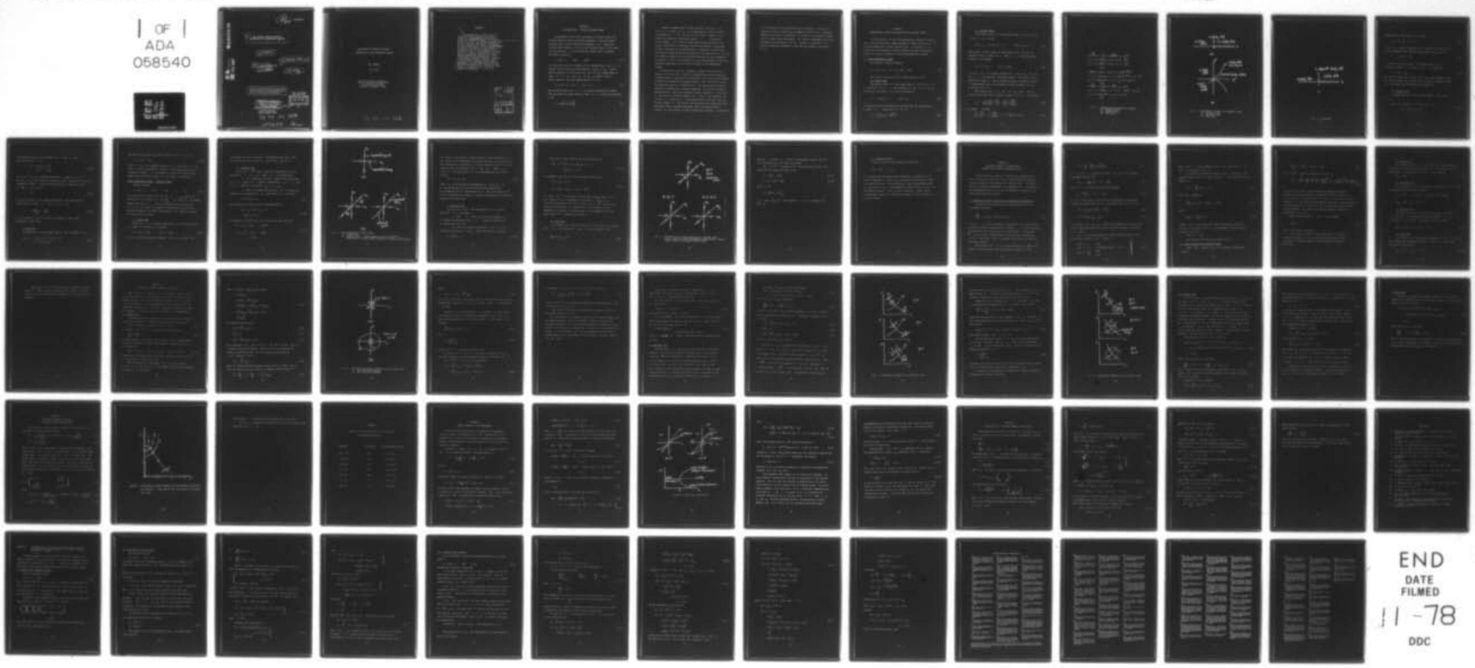

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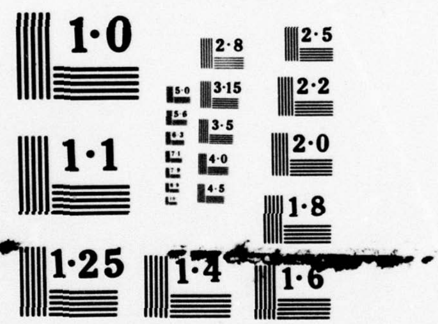

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6 RELAXATION AT CRITICAL POINTS:
DETERMINISTIC AND STOCHASTIC THEORY.

10 Marc Mangel

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RELAXATION AT CRITICAL POINTS:

DETERMINISTIC AND STOCHASTIC THEORY

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June 1978

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ABSTRACT

A generalized critical point is characterized by totally non-linear dynamics. ~~We formulate~~ the deterministic and stochastic theory of relaxation is formulated at such a point. Canonical problems are used to motivate the general solutions. In the deterministic theory, ~~we show that~~ at the critical point certain modes have polynomial (rather than exponential) growth or decay. The stochastic relaxation rates can be calculated in terms of various incomplete special functions. Three examples are considered. First, a substrate inhibited reaction (marginal type dynamical system). Second, the relaxation of a mean field ferromagnet. ~~We obtain~~ a result is obtained that generalizes the work of Griffiths et al. Third, ~~we consider~~ the relaxation of a critical harmonic oscillator is considered.

SECTION 1

INTRODUCTION: "CRITICAL SLOWING DOWN"

Thermodynamic and kinetic generalized critical points are characterized by totally non-linear dynamics. Such non-linear dynamics lead to many interesting phenomena, e.g., "anomalous" fluctuations (treated in (1)) and the "slowing" down of the decay of a perturbation. To illustrate the latter effect, consider the kinetic equation:

$$\dot{x} = b(x, \alpha) \qquad x \in R^1 \qquad \alpha \in R^{\psi j} \tag{1.1}$$

for which the origin is assumed to be a steady state: $b(0, \alpha) = 0$. Suppose that the system is perturbed to a value $x = x_0$. A well defined problem is to calculate the time that the system takes to reach $\delta (0 < \delta << x_0)$ from x_0. If x_0 is "small," then a natural approach involves approximating (1.1) by

$$\dot{x} = b'(0, \alpha)x + 0(x^2) \qquad x(0) = x_0. \tag{1.2}$$

Now we assume that $b'(0, \alpha) < 0$, so thatthe perturbation decays. The time that the system takes to reach $x = \delta$ is easily calculated to be

$$t_\delta = \frac{1}{b'(0, \alpha)} \ln\left[\frac{\delta}{x_0}\right] \tag{1.3}$$

However, suppose that for some critical value of $\alpha = \alpha_c$, $b'(0, \alpha_c) = 0$. Then $(0, \alpha_c)$ is a "generalized critical" point: the dynamics at $\alpha = \alpha_c$ are totally non-linear. Equation (1.3) yields the physically ridiculous result $t_\delta = \infty$. Furthermore, (1.2) becomes $\dot{x} = 0$. Both of these difficulties are due to improper linearization procedures, and not any physical divergences. In fact, the decay of the perturbation is algebraic in time, with the exact form determined by the nature of the singularity at $(0, \alpha_c)$. Such simple problems and the canonical bifurcations are considered in section 2. The points essential to the understanding of critical relaxation phenomena can be gained by study of one-dimensional systems.

If fluctuations are not included, a steady state can not be attained in finite time. Since the deterministic forces vanish as a steady state or equilibrium is approached, the ratio of fluctuation intensity to deterministic dynamics grows. Thus, the proper theory of relaxation must be a stochastic one. The deterministic kinetic equation is modified by a Langevin approach. We use the diffusion approximation to treat the stochastic kinetic equation. In particular, we derive a diffusion equation for $T(x'|x)$, the expected time to reach x', starting at x and conditioned on the fact that the process reaches x'. We analyze the one-dimensional equations fully and obtain certain special functions, which are genearlized in section 4 to the solution of multi-dimensional problems. In sections

5-7, we consider three applications of the theory. In section 5, relaxation from a steady state of marginal stability in a substrate inhibited reaction is considered. In section 6, we consider relaxation of a mean field ferromagnet. Our results complement and extend the results of Griffiths et al (2). Finally, in section 7, we discuss relaxation phenomena in the critical harmonic oscillator (1, 3).

SECTION 2

DETERMINISTIC THEORY OF RELAXATION AT CRITICAL POINTS

In this section, we give the deterministic theory of relaxation. Our classification scheme extends the ideas of Kubo et al (4) to multi-dimensional systems (section 2.2). In section 2.1, we stress the one-dimensional results, because the multi-dimensional theory is a natural extension of the one-dimensional results.

2.1 ONE-DIMENSIONAL SYSTEMS

We consider a kinetic equation

$$\dot{x} = b(x, \alpha_c) \quad x(0) = x_0 \quad x \in R^1 \quad \alpha \in R^n. \tag{2.1}$$

The origin is assumed to be a steady state of (2.1).

A. Normal Type

The steady state is of the normal type if $b'(0, \alpha) \neq 0$. It is stable if $b'(0, \alpha) < 0$ and unstable if $b'(0, \alpha) > 0$. In the vicinity of the origin, (2.1) can be replaced by

$$\dot{x} = b'(0, \alpha)\, x \qquad x(0) = x_0 \tag{2.2}$$

As mentioned in the introduction, the time that the system takes to reach $x = \delta$, starting at $x = x_0$ is

$$t_\delta = \frac{1}{|b'(0, \alpha)|} \ln\left[\frac{x_0}{\delta}\right]. \tag{2.3}$$

B. Marginal Type

The steady state is of the marginal type if $\alpha \in R^1$ and for a value $\alpha = \alpha_c$ we have

$$b(0, \alpha_c) = b'(0, \alpha_c) = 0 , \qquad b''(0, \alpha_c) \neq 0 \tag{2.4}$$

There exists a local change of coordinates (e.g., (5),(6), or Appendix A here) so that for α near α_c , x near the origin equation (2.1) becomes

$$\dot{y} = y^2 - \beta(\alpha) , \qquad y(0) = y_0(x_0) \tag{2.5}$$

In (2.5), $\beta(\alpha)$ is a regular function of α and $\beta(\alpha_c) = 0$. We call $\alpha = \alpha_c$ the marginal bifurcation point. The flow of (2.5) is sketched in figure 1. The bifurcation picture is shown in figure 2. The marginal case was considered briefly by Kubo et al (4) and Nitzan et al (7).

Now suppose that $\beta > 0$ and $-\sqrt{\beta} < y_o < \sqrt{\beta}$. One can calculate the time that it takes to reach $y_1 = -\sqrt{\beta} + \delta$. We obtain

$$t_{y_1} = \frac{1}{2\sqrt{\beta}} \left\{ \ln\left\{\frac{y_1 - \sqrt{\beta}}{y_1 + \sqrt{\beta}}\right\} - \ln\left\{\frac{y_0 - \sqrt{\beta}}{y_0 + \sqrt{\beta}}\right\} \right\} \tag{2.6}$$

For small we have

$$\frac{y_1 - \sqrt{\beta}}{y_1 + \sqrt{\beta}} = \frac{1 - \sqrt{\beta}/y_1}{1 + \sqrt{\beta}/y_1} = (1 - \sqrt{\beta}/y_1)^2 + 0(\beta) \tag{2.7}$$

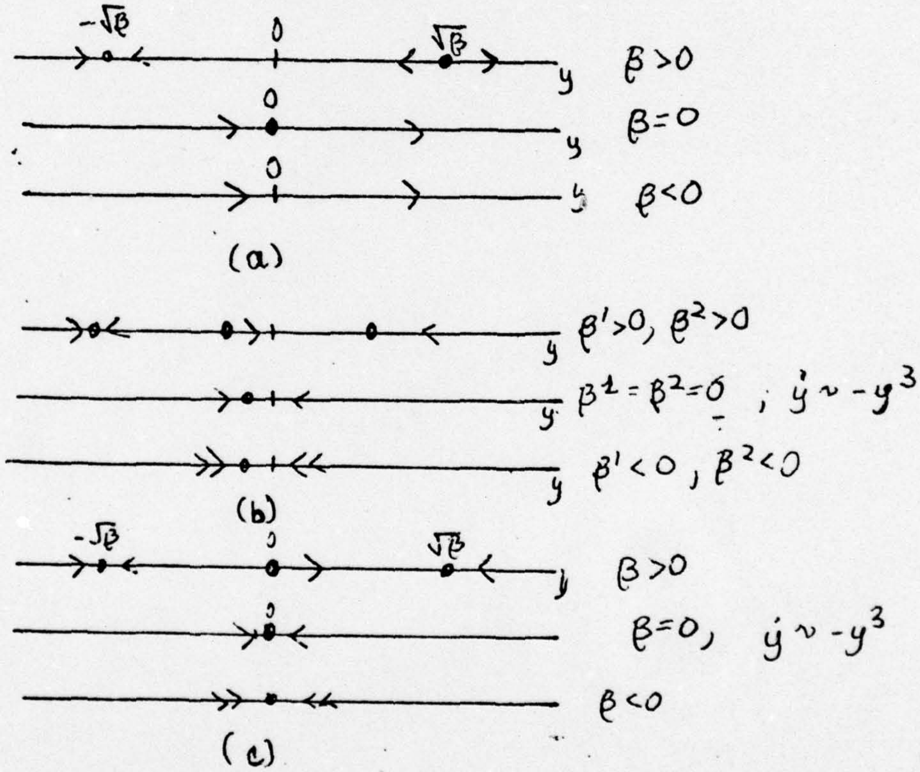


FIG. 1: DYNAMICS OF THE CANONICAL SYSTEMS
(a) MARGINAL TYPE
(b) CRITICAL TYPE
(c) HOPF TYPE

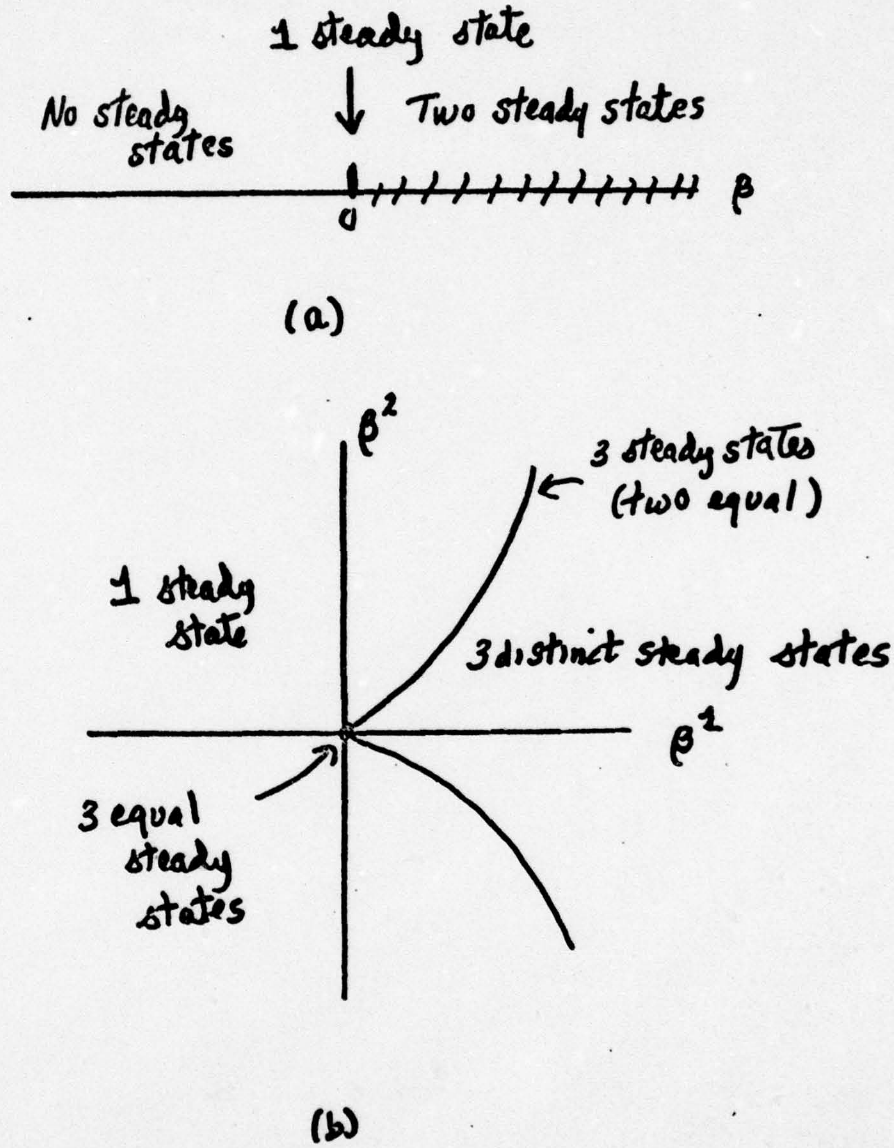
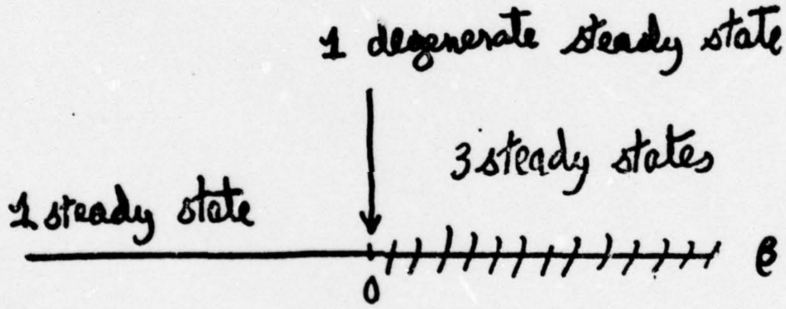


FIG. 2: BIFURCATION PICTURES IN PARAMETER SPACE
(a) MARGINAL TYPE;
(b) CRITICAL TYPE;
(c) HOPF TYPE



(c)

FIG. 2: (Continued)

Expanding the logarithms in (2.6) gives

$$t_{y_1} \sim \frac{1}{y_0} - \frac{1}{y_1} + 0(\beta) \tag{2.8}$$

so that t_{y_1} remains finite as $\beta \to 0$. Clearly, this result would not be obtained had we used the linearized version of (2.5):

$$y' = -2\sqrt{\beta}\,(y + \sqrt{\beta}) \tag{2.9}$$

In another possible situation $\beta=0$. Suppose that $y_0 < 0$. The time to reach $\delta < 0$ from y_0 $(y_0 < \delta)$ is (exactly)

$$t = -\frac{1}{\delta} + \frac{1}{y_0} \tag{2.10}$$

The point of importance is that (2.8, 2.9) yield algebraic forms for the relaxation time, whereas (2.3) yields a logarithmic time (i.e., algebraic versus exponential relaxation).

C. Critical Type

A steady state is of the critical type if $\alpha \in R^2$ and for $\alpha = \alpha_c$

$$\begin{gathered} b(0, \alpha_c) = b'(0, \alpha_c) = b''(0, \alpha_c) = 0 \\ b'''(0, \alpha_c) \neq 0 \end{gathered} \tag{2.11}$$

The canonical form of the dynamics, for α near α_c and y near 0 is (for $b''' < 0$)

$$\dot{y} = -y^3 + \beta^1(\alpha)y + \beta^2(\alpha)$$
$$y(0) = y_0(x_0) \tag{2.12}$$

In (2.12), $\beta(\alpha)$ is a regular function of α and $\beta(\alpha_c) = 0$. We call $\alpha = \alpha_c$ the critical bifurcation point. The flow of (2.12) is sketched in figure 1. The bifurcation picture is shown in figure 2. When $\alpha = \alpha_c$, we have

$$\dot{y} = -y^3 \tag{2.13}$$

so that the origin is very weakly attracting. The time that the system takes to reach $y = \delta$ from $y = y_1 > \delta$ is

$$t_\delta = -\frac{1}{2}\left[\frac{1}{y_1^2} - \frac{1}{\delta^2}\right] \tag{2.14}$$

As in the marginal case, we obtain an algebraic, rather than exponential, decay rate.

D. Hopf Type

A steady state is of the Hopf type if $\alpha \in R^1$ and when $\alpha = \alpha_c$

$$b(0, \alpha_c) = b'(0, \alpha_c) = b''(0, \alpha_c) = 0$$
$$b'''(0, \alpha_c) \neq 0 \tag{2.15}$$

The canonical dynamics (8) in this case (for $b''' < 0$) are

$$\dot{y} = -y(y^2 - \beta(\alpha)) \tag{2.16}$$

where $\beta = \beta(\alpha)$ is a regular function of α and $\beta(\alpha_c) = 0$. The flow of (2.16) is sketched in figure 1. The bifurcation picture is sketched in figure 2. It is important to note the difference between Hopf and critical cases (i.e. the number of parameters).

MULTI-DIMENSIONAL THEORY: CANONICAL FORMS

We now consider

$$\dot{x} = b(x, \alpha) \qquad x \in R^n \qquad \alpha \in R^1 \qquad \text{or} \qquad R^2 \tag{2.17}$$

with the origin a steady state. We let $\lambda_1, \ldots, \lambda_n$ denote the eigenvalues of the matrix $B = (b^i{}_{,j})\Big|_0$. For simplicity, we assume assume that there are n distinct eigenvalues and eigenvectors. Let k_+, k_-, k_0 denote the number of eigenvalues with real part positive, negative, and zero, respectively. The dynamical systems are classified as follows.

A. Normal Case

Hence $k_0 = 0$. It is well known that (2.17) can be replaced by a change of variables $x \to y$ so that

$$\dot{y}^i = \lambda_j y^i + 0(y^2) \qquad y^i(0) = y^i(x_0) \tag{2.18}$$

If $k_+ = 0$, then the origin is stable. If $k_+ > 0$, then R^n can be divided into two sub-spaces: an expanding part (W_e), and a contracting part (W_c) (figure 3), with $\dim W_e + \dim W_c = n$.

B. Marginal Case

We now let $\alpha \in R^1$ vary. Then the eigenvalues of B are functions of α: $\lambda_k = \lambda_k(\alpha)$. When $\alpha = \alpha_c$ we assume that,

1) All eigenvalues are real. Exactly one eigenvalue $\lambda_0(\alpha_c) = 0$. There are k negative eigenvalues, $\lambda_1, \ldots, \lambda_k$ and $n - 1 - k$ positive eigenvalues $\lambda_{k+1}, \ldots, \lambda_{n-1}$.

2) There are enough eigenvectors. Let Z denote the eigenvector corresponding to λ_0. Then from (2.17), we obtain,

$$\dot{Z} = \tilde{b}(y(Z), \alpha) \tag{2.19}$$

The marginal type steady state is characterized by

$$\begin{aligned} &\tilde{b}(0, \alpha_c) = \tilde{b}_Z(0, \alpha_c) = 0 \\ &\tilde{b}_{ZZ}(0, \alpha_c) \neq 0 \end{aligned} \tag{2.20}$$

In appendix A, we show that (2.17) can be put into the form

$$\begin{aligned} \dot{y}^i &= \lambda_i y^i + 0(y^2) \qquad && y^i \in R^{n-1} \\ \dot{y}^0 &= (y^0)^2 \pm \beta(\alpha) && y^0 \in R^1 \\ &\quad + 0(y^3) \end{aligned} \tag{2.21}$$

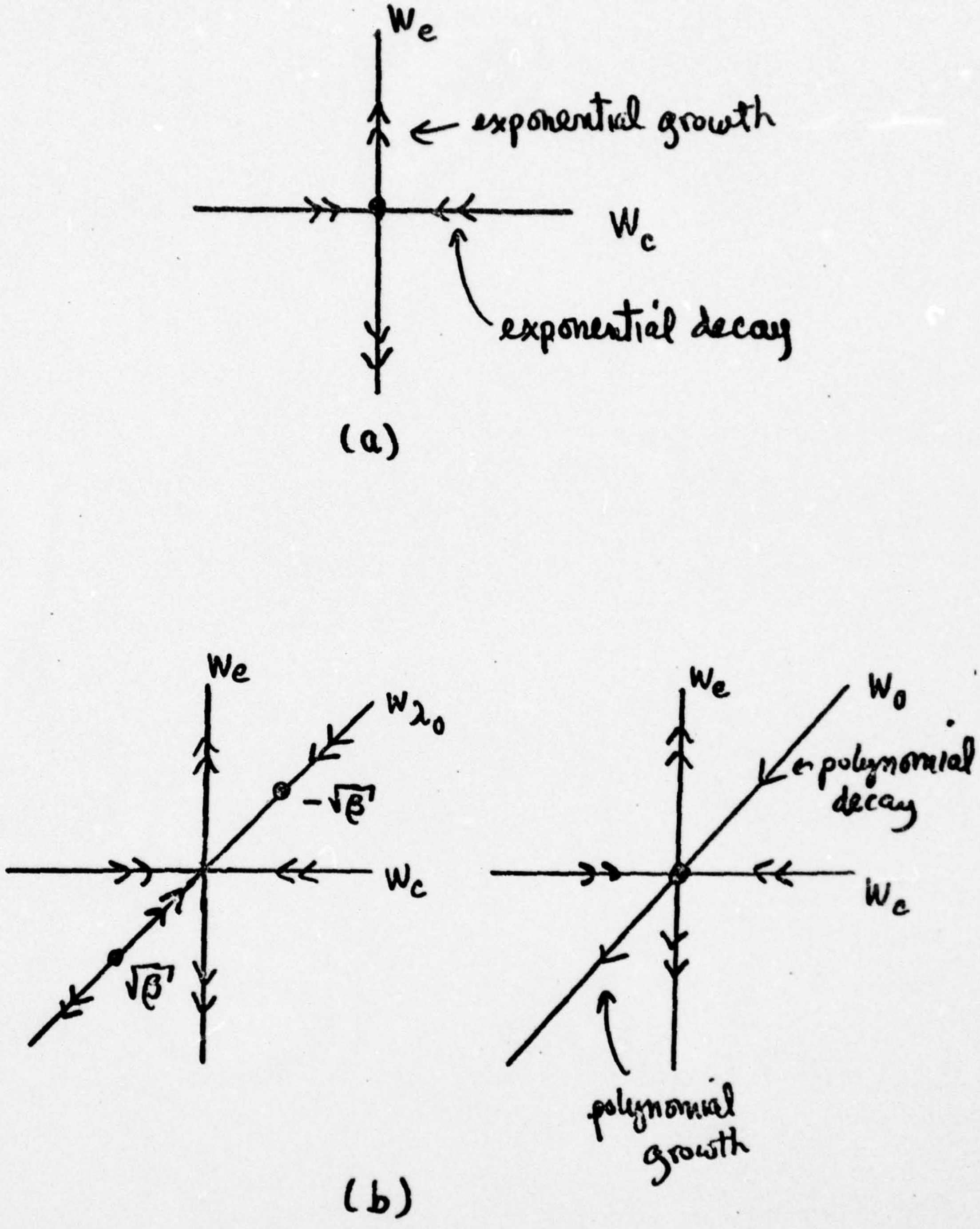


FIG. 3: MULTI-DIMENSIONAL PHASE SPACES.
(a) NORMAL TYPE
(b) MARGINAL TYPE: DOUBLE ARROWS INDICATE EXPONENTIAL GROWTH/DECAY; SINGLE ARROWS INDICATE POLYNOMIAL GROWTH/DECAY

Our result is approximate, whereas Arnold (5) and Shoshaitshvili (6) show there exist transformations which eliminate the higher terms. The construction in appendix A is useful, however, in that it gives explicit ways of calculating the y and $\beta(\alpha)$. When $\alpha = \alpha_c$, $\beta(\alpha_c) = 0$. The phase space R^n is now decomposed into a direct product

$$R^n = W_0 + W_e + W_c \tag{2.22}$$

where W_0 is the manifold corresponding to λ_0 and W_e, W_c are the expanding and contracting sub-spaces respectively. The assumption that all eigenvalues of B were real affected the form of the canonical equations. Complex eigenvalues are explicitly treated in the Hopf case.

C. Critical Type

In this case, $\alpha \in R^2$. The eigenvalues of B are still denoted by $\lambda(\alpha)$. We assume:

1) When $\alpha = \alpha_c$ there is one zero eigenvalue, λ_0, k negative eingenvalues and $n - k - 1$ positive eigenvalues. All eigenvalues are real.

2) There are enough eigenvectors. Let Z be the eigenvector belonging to $\lambda_0(\alpha)$. Then from (2.17), we obtain

$$\dot{Z} = \tilde{b}(y(Z), \alpha) \tag{2.23}$$

The critical type steady state is characterized by

$$\tilde{b}(0, \alpha_c) = \tilde{b}_Z(0, \alpha_c) = \tilde{b}_{ZZ}(0, \alpha_c) = 0$$

$$\tilde{b}_{ZZZ}(0, \alpha_c) \neq 0 \tag{2.24}$$

In appendix A, we show that the canonical dynamics are

$$\dot{y}^i = \lambda_i y^i + 0(y^2)$$

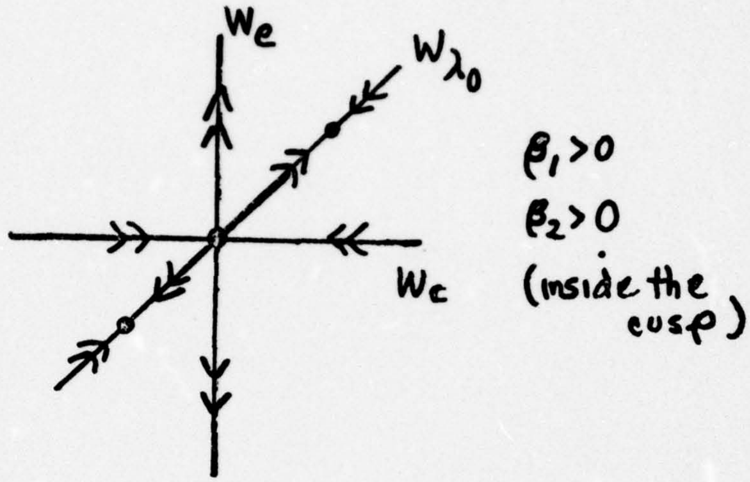
$$\dot{Z} = \pm(Z^3) - \beta_1(\alpha)Z - \beta_2(\alpha) + 0(Z^4) \tag{2.25}$$

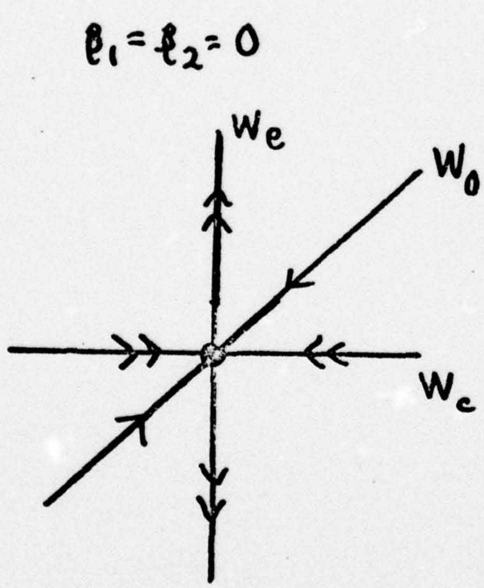
In (2.25), $\beta(\alpha)$ is a regular function that vanishes when $\alpha = \alpha_c$ The $\pm$ sign in (2.25) corresponds to the sign of $\tilde{b}_{ZZZ}(0, \alpha_c)$. Arnold and Shoshaitshvili state a theorem in which the higher order terms are eliminated. As remarked above, the constructions in appendix A are useful for applications. The decomposition of the phase space R^n is sketched in figure 4.

D. Hopf Type

In the Hopf case, $\alpha \in R^1$ and some of the eigenvalues are complex. When $\alpha = \alpha_c$ one eigenvalue, $\lambda_0(\alpha)$ is a pure imaginary with

$$\frac{d}{d\alpha} \mathrm{Re}\lambda_0(\alpha) \Big|_{\alpha_c} \neq 0 \tag{2.26}$$





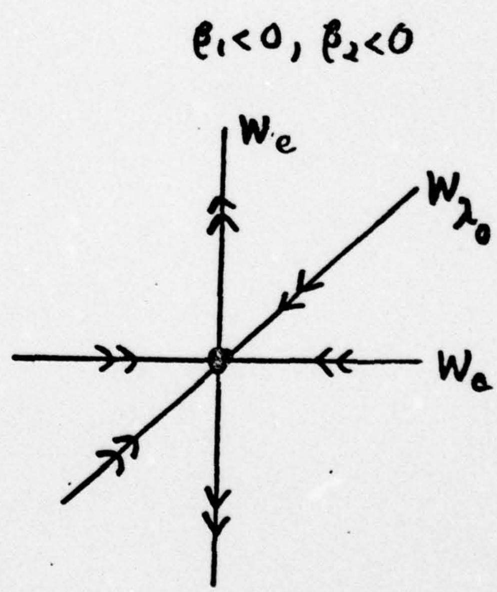


FIG. 4: DECOMPOSITION OF PHASE SPACE IN THE CRITICAL CASE. DOUBLE ARROWS INDICATE EXPONENTIAL GROWTH/DECAY. SINGLE ARROWS INDICATE POLYNOMIAL GROWTH/DECAY.

Thus, as α crosses α_c, a pair of eigenvalues closses from the left half plane into the right half plane.

Let $x = re^{i\theta}$. Fenichel (1975) (also see Arnold (1972)) has shown that the canonical dynamics are

$$\dot{r} = \pm(b_1 r^3 - \eta \gamma_1 r) \tag{2.27}$$

$$\dot{\theta} = \lambda_2 + b_2 r^2 + \eta \gamma_1 r \tag{2.28}$$

where γ_1 is

$$\gamma_1 = \frac{d}{d\alpha} \operatorname{Re} \lambda_i(\alpha) \Big|_{\alpha_c} ,$$

$\lambda_2 > 0$ and $b_1, b_2 \neq 0$. The function $\eta = \eta(\alpha)$ is regular and $\eta(0) = 0$.

E. Relaxation Rates

Given an initial displacement from the origin

$$y(0) = \{y_0, \ldots, y_{n-1}\} \tag{2.25}$$

it is clear that the appropriate relaxation (or growth) rate of the k^{th} component (or mode) can be explicitly calculated by using the canonical forms. The calculations reveal exponential growth in W_e, decay in W_c, and polynomial growth or decay in W_0 (at bifurcation points). Thus, we have a complete, albeit local, deterministic theory for relaxation phenomena in the vicinity of critical points.

SECTION 3

STOCHASTIC THEORY OF RELAXATION: FORMULATION AND ONE-DIMENSIONAL RESULTS

The deterministic theory of section 2 is approximate in that it ignores fluctuations. Since the deterministic dynamics vanish (to perhaps second order) at a steady state, the proper theory of relaxation phenomena is a stochastic one. Our theory is still phenomenological, but it may be possible to connect it to underlying statistical physics.

3.1 STOCHASTIC KINETIC EQUATION AND DIFFUSION APPROXIMATION

We replace the deterministic kinetic equation (2.17) by the Langevin equation:

$$\frac{d\tilde{x}^i_\tau}{dt} = b^i(\tilde{x}_\tau) + \frac{\sqrt{\varepsilon}}{\tau}\,\sigma^i_j(x)\,\tilde{y}^j(t/\tau) \tag{3.1}$$

In (3.1), τ is a small parameter relating the time scales of the fluctuations and the deterministic dynamics, ε is a small parameter characterizing the intensity of the fluctuations. The process $\tilde{y}^j$ is a zero mean, mixing process (for more exact assumptions, see (9)). The field $\sigma^i_j(x)$ is assumed to be known, or given by some prescription.

The process $\tilde{y}(S)$ in (3.1) has correlations. Hence, our model is more reasonable than "white noise" models. We let

$$\gamma^{kl} = \int_0^\infty E\left[\tilde{y}^k(S)\tilde{y}^l(0)\right] ds \tag{3.2}$$

As $\tau \to 0$, $x_\tau \to x$, a diffusion process. If $u_0(x)$ is a bounded, measurable function and

$$u(x, t) = E\left\{u_0(\tilde{x}(t)) \,|\, \tilde{x}(0) = x\right\}, \tag{3.3}$$

then $u(x, t)$ satisfies the backward equation

$$u_t = \frac{\varepsilon a^{ij}}{2} u_{ij} + (b^i + \varepsilon c^i) u_i . \tag{3.4}$$

In (3.4), subscripts indicate partial differential and repeated indices are summed from 1 to n. The coefficients a^{ij}, c^i are

$$a^{ij} = \sigma^i_k(x)\sigma^j_l(x) \left[\gamma^{kl} + \gamma^{lk}\right] \tag{3.5}$$

$$c^i = \gamma^{kl}\sigma^j_k(x) \frac{\partial}{\partial x^i} \sigma^i_l(x) \tag{3.6}$$

In practice $a(x)$ and $c(x)$ cannot be calculated from first principles, but some prescription must be given for their calculation (e.g., (10)).

Let N be a neighborhood of a stable steady state or, more generally, a domain in R^n. We set

$$\left.\begin{aligned} &u(x, t) = 1 && x \in N \\ &u(x, t) \to 0 && \text{as distance from } x \text{ to } N \to \infty \\ &u(x, 0) = \begin{cases} 0 & x \notin N \\ 1 & x \in N \end{cases} \end{aligned}\right\} \tag{3.7}$$

Then, $u(x, t)$ is the probability that $\tilde{x}(t)$ has entered N by time t, given that $\tilde{x}(0) = x$.

For stochastic relaxation theory, we are interested in the expected time to enter N, given $\tilde{x}(0) = x$ and that the process enters N:

$$T(x) = \int_0^\infty t u_t(x, t)\, dt. \tag{3.8}$$

Then $T(x)$ satisfies

$$\frac{\varepsilon a^{ij}}{2} T_{ij} + (b^i + \varepsilon c^i) T_i = -\bar{u}(x) \tag{3.9}$$

where

$$\bar{u}(x) = \lim_{t \to \infty} u(x, t) \tag{3.10}$$

Namely, $\bar{u}(x)$ is the probability that the process eventually enters N, given that $\tilde{x}(0) = x$. The boundary conditions appropriate to (3.9) are

$$\begin{gathered} T(x) = 0 \qquad x \in N \\ \text{and a growth condition as distance } (x, N) \to \infty \end{gathered} \tag{3.11}$$

3.2 EXACT SOLUTION AND CANONICAL FORMS

When $x \in R^1$, equation (3.9) is an ordinary differential equation

$$\frac{\varepsilon a}{2} T_{xx} + (b(x) + \varepsilon(c))T_x = -\bar{u}(x) \tag{3.12}$$

Let $N = \{\hat{x}\}$. Then the solution of (3.12) is

$$T(x) = \int_x^{\hat{x}} \frac{a}{\varepsilon} \exp\left[-\frac{2}{\varepsilon}\int^s \frac{b+\varepsilon c}{a}\, dy\right] \int_{-\infty}^{s} \bar{u}(x) \exp\left[\frac{2}{\varepsilon}\int^{x'} \frac{b+\varepsilon c}{a}\, dy\right] dx'\, ds \tag{3.13}$$

Equation (3.13) has a rather conplicated asymptotic analysis. Instead of doing an asymptotic analysis on (3.13), we return to (3.12) and set, for convenience $a \equiv 2$, $\bar{u}(x) \equiv 1$, and $c=0$. We will analyze (3.12) and obtain certain special functions. These functions will be generalized in section 4, for the solution of multi-dimensional problems. Our analysis is based on matched asymptotic expansions (e.g., (11)).

Away from the zeros of $b(x)$, (3.12) becomes

$$b(x)T_x = -1 \tag{3.14}$$

This is the "outer" equation.

Near zeros of $b(x)$, (3.14) breaks down. We need to stretch coordinates (3.12) to obtain the appropriate "inner" equations. We shall analyze (3.12) by using the canonical form of $b(x)$.

A. Normal Case

In the normal case, $b(x) = \pm x$, with (+) indicating that the origin is an unstable steady state, (-) indicating a stable steady state. Introducing $z = x/\sqrt{\varepsilon}$, (3.12) becomes

$$T_{zz} \pm zT_z = -1 \tag{3.15}$$

B. Marginal Case

In the marginal case, the canonical dynamics are $b(x) = \pm(x^2) - \tilde{\alpha}$. We introduce the stretched variables

$z = x/\varepsilon^{1/3}$, $\alpha = \tilde{\alpha}/\varepsilon^{2/3}$, so that (3.12) becomes

$$T_{zz} \pm (z^2 - \alpha)T_z = -1/\varepsilon^{1/3} \tag{3.16}$$

C. Critical Case

In the critical case, the canonical dynamics are $b(x) = \pm x^3 + \tilde{\beta}_1 x + \tilde{\beta}_2$. We introduce stretched variables $z = x/\varepsilon^{1/4}$, $\beta_1 = \tilde{\beta}_1/\varepsilon^{1/2}$, $\beta_2 = \tilde{\beta}_2/\varepsilon^{3/4}$ and obtain the inner equation

$$T_{zz} + (\pm z^3 + \beta_1 z + \beta_2)T_z = -1/\varepsilon^{1/2} \tag{3.17}$$

D. Hopf Case

In the Hopf case, the canonical dynamics are $b(x) = -x^3 + \tilde{\beta}x$. We introduce the stretched variables $z = x/\varepsilon^{1/4}$, $\beta = \tilde{\beta}/\varepsilon^{1/2}$ and obtain the inner equation

$$T_{zz} + (-z^3 + \beta z)T_z = -1/\varepsilon^{1/2} \tag{3.18}$$

Equations (3.15-3.18) define certain incomplete special functions. These special functions will be used in the next section to construct asymptotic solutions of multi-dimensional problems.

SECTION 4

STOCHASTIC THEORY: ASYMPTOTIC RESULTS

When $x \in R^n$ $n \geq 2$, equation (3.9) will usually not have exact solutions. Consequently, approximate techniques are required. The methods used here are closely related to those in (10). The basic idea is to generalize the one-dimensional inner solutions; we call the method a generalized ray method. Although the normal case does not represent a "critical" point, we include it for completeness.

4.1 NORMAL CASE

We suppose that the origin is a simple steady state (figure 5) and that it is stable. We seek a solution of (3.9) in the form

$$T(x) = g(x)F(\psi/\sqrt{\varepsilon}) + h(x)\varepsilon^{\frac{1}{2}} F'(\psi/\sqrt{\varepsilon}) + k(x) . \tag{4.1}$$

In equation (41.), F(z) is a special function satisfying

$$\frac{d^2F}{dz^2} = z\frac{dF}{dz} - 1 \tag{4.2}$$

and the functions $\psi(x)$, $g(x)$, $h(x)$, and $k(x)$ are to be determined. In order to completely analyze the problem, we assume that g, h, k have expansions

$$g(x) = \Sigma\, g^n(x)\varepsilon^n \qquad h(x) = \Sigma\, h^n(x)\varepsilon^n \qquad k(x) = \Sigma\, k^n(x)\varepsilon^n \tag{4.3}$$

Consequently, the construction given here represents the first term in the asymptotic solution of (3.9).

When derivatives are evaluated, (4.2) is used to replace $F''(\psi/\sqrt{\varepsilon})$ by $\psi/\sqrt{\varepsilon}\, F'(\psi/\sqrt{\varepsilon}) - 1$. Then terms are collected according to powers of ε. We obtain:

$$
\begin{aligned}
-\bar{u}(x) = {} & \epsilon^{-\frac{1}{2}} \left[b^i \psi_i + \frac{a^{ij}}{2} \psi_i \psi_j \psi\right] (g+h\psi)F' \\
& + \epsilon^0 F(b^i g_i) \\
& + \epsilon^0 (b^i k_i + \frac{a^{ij}}{2} \psi_i \psi_j g) \\
& + \epsilon^{\frac{1}{2}} F' \Big[b^i h_i + \frac{a^{ij}}{2} g\psi_j + a^{ij} h_i \psi_j \psi \\
& + \frac{a^{ij}}{2} h\psi_{ij}\psi + \frac{a^{ij}}{2} \psi_i \psi_j h - gc^i \psi_i \\
& + hc^i \psi_i \psi\Big]
\end{aligned}
\tag{4.4}
$$

The leading terms vanish if

$$b^i \psi_i + \frac{a^{ij}}{2} \psi_i \psi_j \psi = 0 \tag{4.5}$$

$$b^i g_i = 0 \tag{4.6}$$

$$b^i k_i + \frac{a^{ij}}{2} \psi_i \psi_j g = -\bar{u}(x) \tag{4.7}$$

First consider (4.5). Since $b^i(0) = 0$ for all i, we set $\psi(0) = 0$, in order to keep $\psi(x)$ regular. Then (4.5) can be solved by the method of characteristics. We note that the transformation $\Phi = \frac{1}{2}\psi^2$ converts (4.5) to

$$b^i \Phi_i + \frac{a^{ij}}{2} \Phi_i \Phi_j = 0 \ , \tag{4.8}$$

which is a Hamilton-Jacobi equation (see also (12)). Then, we can solve the Hamilton-Jacobi equation in terms of characteristics:

$$\dot{x}^i = \frac{\partial H}{\partial p_i} \qquad \dot{p}^i = \frac{-\partial H}{\partial x^i} \qquad \dot{\Phi} = \frac{1}{2} a^{ij} p_i p_j \tag{4.9}$$

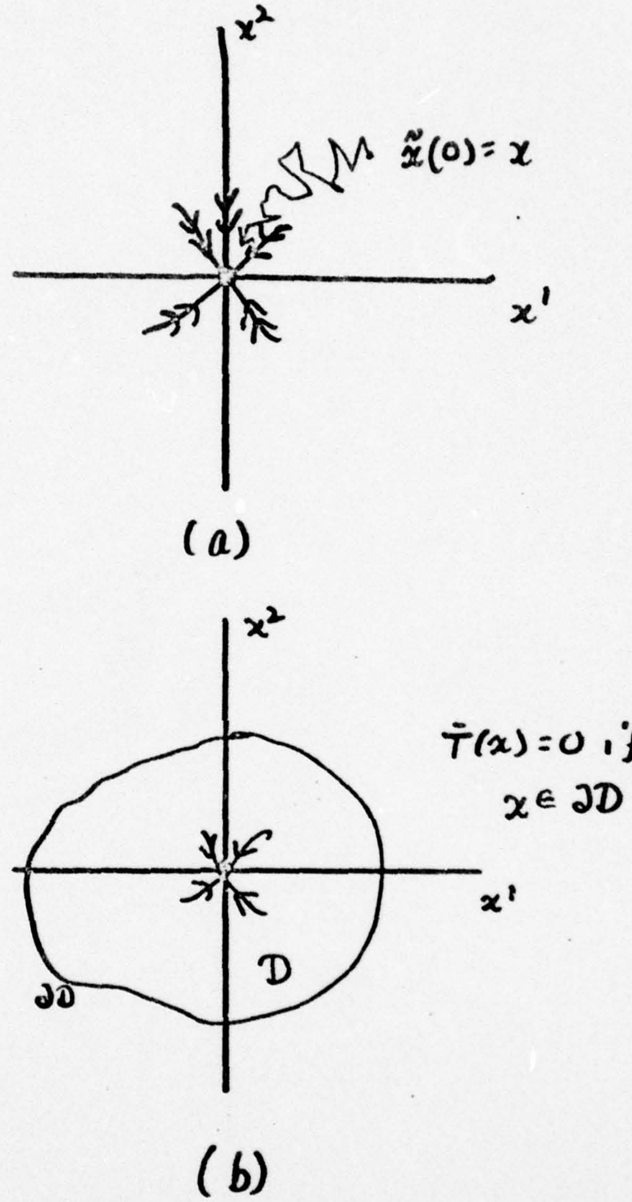


FIG. 5: STOCHASTIC RELAXATION PROBLEMS IN THE NORMAL CASE.
(a) THE RELAXATION PROBLEM
(b) THE FIRST EXIT PROBLEM

where

$$H(x, p) = b^i p_i + \frac{a^{ij}}{2} p_i p_j \tag{4.10}$$

Starting at the origin, the phase plane is covered with trajectories, called rays, along which ψ (or Φ) is known. Thus, ψ at any point x is known.

Equation (4.3) indicates that g is constant on deterministic trajectories. Since all trajectories intersect at the origin, g must have the same value on all trajectories. At the origin, (4.7) becomes

$$\frac{a^{ij}}{2} \psi_i \psi_j g = -\bar{u}(0) = -1 \tag{4.11}$$

Thus

$$g = \frac{-1}{\frac{a^{ij}}{2} \psi_i \psi_j} . \tag{4.12}$$

We set $k(0) = 0$ as initial data for (4.7).

If we set $F(0) = F'(0) = 0$ as initial conditions in (4.2), then the leading term of the asymptotic solution satifies $T(0) \equiv 0$.

The $0(\varepsilon^{1/2}F')$ term in (4.4) vanishes if

$$\begin{aligned} b^i h_i + \frac{a^{ij}}{2} g\psi_{ij} + a^{ij} h_i \psi_j \psi + \frac{a^{ij}}{2} h\psi_{ij}\psi \\ + \frac{a^{ij}}{2} \psi_i \psi_j h - gc^i \psi_i + hc^i \psi_i \psi = 0 \end{aligned} \tag{4.13}$$

At the origin $b'(0) = \psi(0) = 0$, so that (4.13) becomes

$$h(0) = \frac{1}{\frac{a^{ij}}{2}\psi_i\psi_j} \left\{ \frac{-a^{ij}}{2} \psi_{ij} g + c^i \psi_i g \right\} \tag{4.14}$$

Equation (4.13) can be solved by the method of characteristics, with initial data given by (4.14).

Thus, we have completely constructed the leading term of the asymptotic solution of (3.9).

As a by-product of our method, we are able to approximately solve the famous Kolmogorov first exit problem, recently considered by Matkowoky and Schuss (13) using matched asymptotic expansions. This problem is the following: suppose that the origin is surrounded by a domain D, with boundary ∂D. Find the expected time that the process takes to hit the boundary (i.e. the mean exit time from D) (Fig. 5b) from x.

We follow the arguments leading to equations (4.1 - 4.11), except that the initial data for F, F' and $k(x)$ change. We set $k(x) \equiv 0$ on ∂D. We distinguish two cases:

i) The boundary ∂D is a contour of ψ (or Φ) say, $\psi = \psi_D$ on ∂D. Then we set

$$F(\psi_D/\sqrt{\varepsilon}) = F'(\psi_D/\sqrt{\varepsilon}) = 0 \tag{4.15}$$

when solving (4.2). Then $T \equiv 0$ on D.

ii) The boundary ∂D is not a contour of ψ. Let ψ_I and ψ_{II} denote the maximum and minimum values of ψ on ∂D. Then $T \not\equiv 0$ on ∂D, but it can be shown that on ∂D

$$|T| \leq |\ell n(\psi_I/\psi_{II})| \tag{4.16}$$

+ exponentially small terms.

Hence, if $|\ell n(\psi_I/(\psi_{II})|$ is small, then $|T(x)|$ will be small on the boundary.

4.2 MARGINAL CASE

In some senses, the marginal case has the least interesting dynamics. The dynamical problem we consider here is sketched on figure 6. When the deterministic system has two nodes (Q_0, Q_1) and one saddle (S), even if the process starts near Q_o, it will eventually reach Q_1, due to the proximity of Q_0 and S. The proper question in the stochastic theory involves the time to cross some given curve R. We note that such a time is infinite in the deterministic case, if the phase point starts on or above S.

We seek a solution of (3.9) of the form

$$T(x) = g(x)B(\psi/\varepsilon^{1/3}, \beta/\varepsilon^{2/3}, 1/\varepsilon^{1/3}, \gamma_2) \tag{4.17}$$

$$+ h(x)\varepsilon^{2/3}B'(\beta/\varepsilon^{2/3}, 1/\varepsilon^{1/3}, \gamma_2) + k(x)$$

In (4.17), $B(z, \alpha, \lambda_1, \lambda_2)$ satisfies

$$\frac{d^2B}{dz^2} = -(z^2 - \alpha)\frac{dB}{dz} - \lambda_1 + \lambda_2 z \tag{4.18}$$

and $g(x)$, $h(x)$, $k(x)$, $\psi(x)$ and the parameters α, γ_2 are to be determined. We proceed as in Section 4.1. Instead of equations (4.5-7) we obtain

$$b^i\psi_i - \frac{a^{ij}}{2}\psi_i\psi_j(\psi^2 - \beta_0) = 0 \tag{4.19}$$

$$b^i g_i = 0 \tag{4.20}$$

$$b^i k_i - \frac{a^{ij}}{2}\psi_i\psi_j g(1 + \gamma_2\psi) = -\bar{u}(x) \tag{4.21}$$

In (4.17), we have set $\beta = \Sigma\beta_k\varepsilon^k$.

We set $\psi^2 = \beta_0$ at Q_0 and at S. In particular $\psi(Q_0) = +\sqrt{\beta_0}$ and $\psi(S) = -\sqrt{\beta_0}$. The value of β_0 can be determined by an iterative procedure (10). We pick an initial value of $\beta_0 = \beta_0^{(0)}$ and solve (4.19) by the method of characteristics, starting at Q_0, where $\psi = \sqrt{\beta_0^{(0)}}$. Some rays will approach S. As a ray approaches S, ψ should approach $-\sqrt{\beta_0^{(0)}}$. If it does not, then the $\beta_0^{(0)}$ must be replaced by a second iterate $\beta_0^{(1)}$. The method of false position

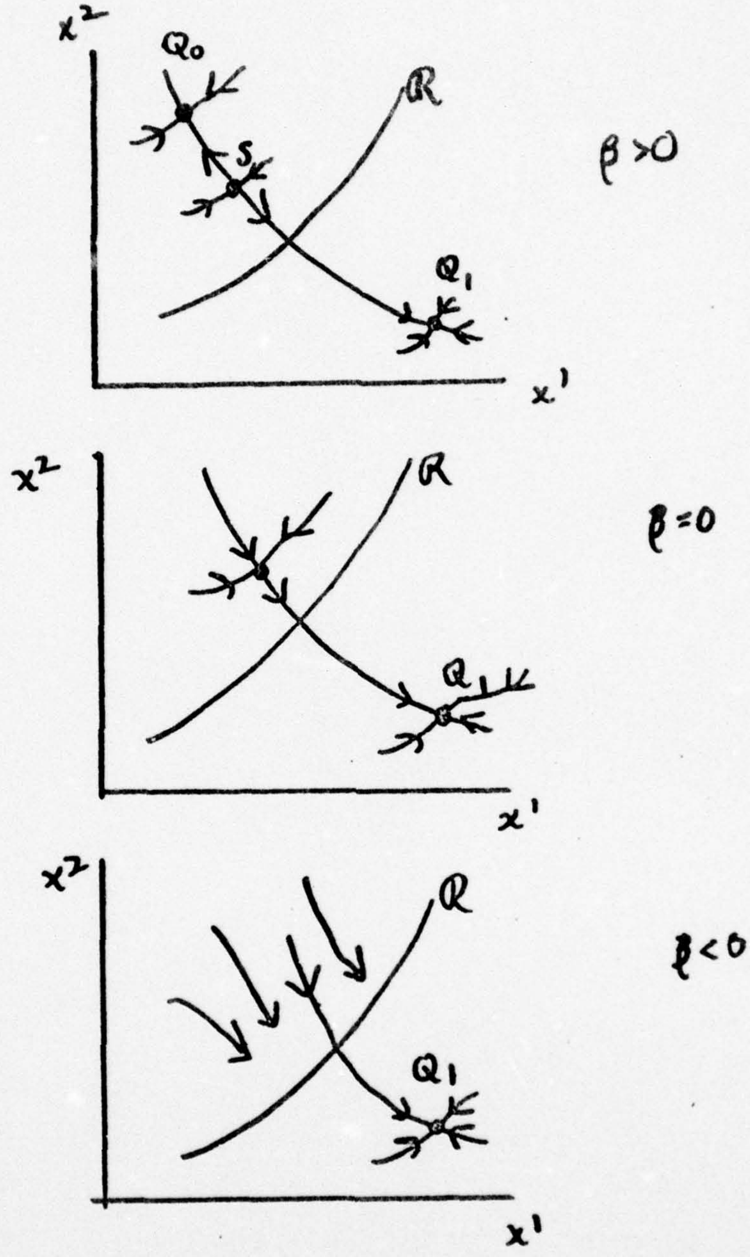


FIG. 6: RELAXATION PROBLEMS IN THE MARGINAL CASE

can be used to calculate iterates of β_0. This procedure can be repeated until β_0 is known to any desired accuracy. (In (10), we present a discussion of this calculation in more detail.)

Equation (4.20) indicates that g is a constant. At Q_0 and Q_1, which we denote generically by P, we have, from (4.21):

$$-\frac{a^{ij}}{2}\psi_i\psi_j\Bigg|_P \quad g(1+\gamma_2\,\psi(P)) = -\bar{u}(P) \tag{4.23}$$

These are two equations for the unknowns g and γ_2. We set $k = 0$ on R and assume that R is a level curve of ψ, with $\psi = \psi_R$ on R. Then we set

$$B(\psi_R/\varepsilon^{1/3},\beta,{}^{1}/\varepsilon^{1/3},\gamma_2) = B^1(\psi_R/\varepsilon^{1/3},\beta,1/\varepsilon^{1/3},\gamma_2) = 0 \tag{4.21}$$

With these choices, $T(x) \equiv 0$ if x R.

At the bifurcation point $\eta = 0$ (the marginal bifurcation) Q_0 and Q_1 coalesce. Then $\beta_0 \equiv 0$, and it can be shown that $\gamma_2 \equiv 0$ (10). At the saddle-node Q_0/Q_1, equation (4.23) still provides one equation for g:

$$g = \frac{\bar{u}(P)}{\frac{a^{ij}}{2}\psi_i\psi_j} \tag{4.24}$$

Elsewhere, we have given proofs that all the construction are regular at the bifurcation point ((10), appendices D, E).

In section 5, we consider an example of a chemical system exhibiting the marginal bifurcation.

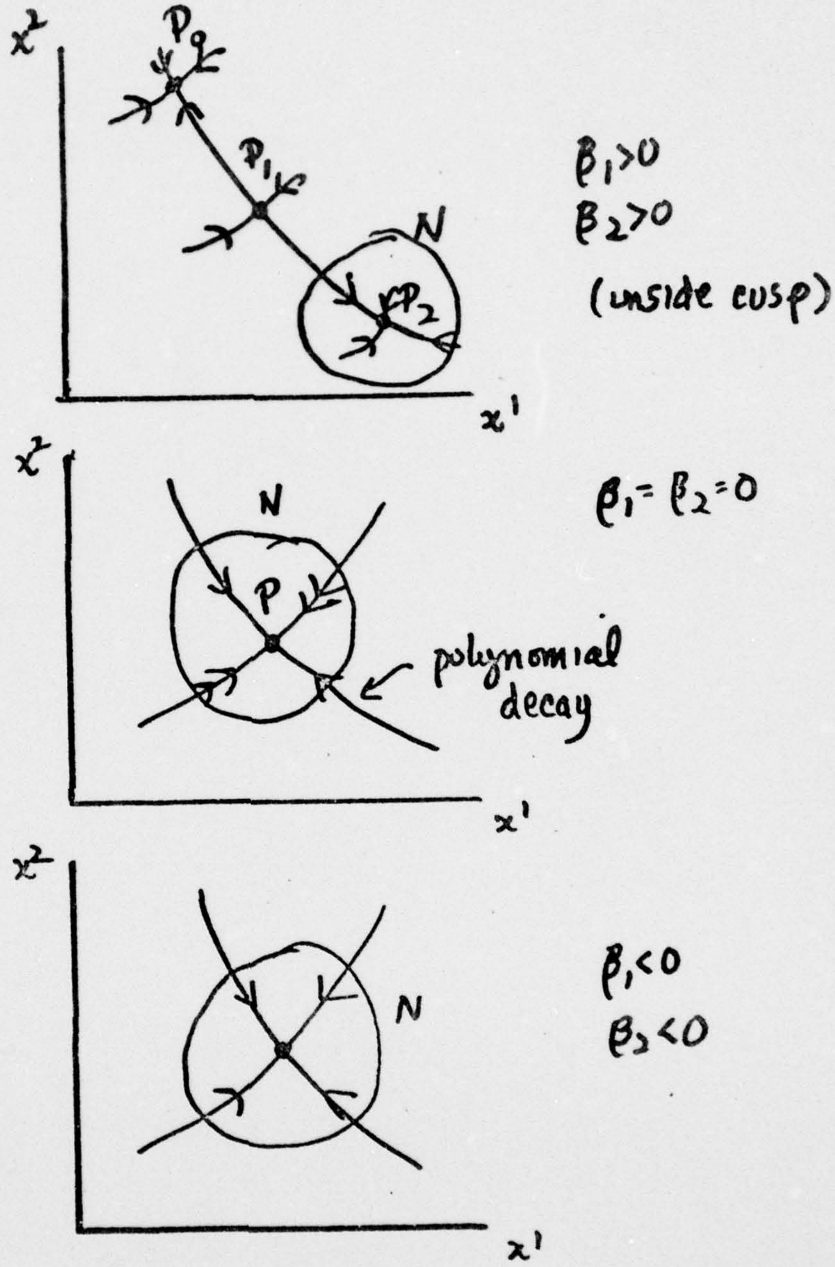


FIG. 7: RELAXATION PROBLEMS IN THE CRITICAL CASE.

4.3 CRITICAL CASE

We now consider a system with three steady states, P_0, P_1, and P_2 when $\alpha_1, \alpha_2 > 0$. When $\alpha_1 = \alpha_2 = 0$ the three steady states coalesce into a critical type steady state. When $\alpha_1, \alpha_2 < 0$ there is only one real steady state; it is assumed to be stable. If $\alpha_1, \alpha_2 > 0$, we surround P_2 by a domain N and pose the following stochastic relaxation problem: what is the expected time to enter N, given the initial position. Clearly there is an analogous problem for a neighborhood N of P_0. When there is only one steady state P, we surround P by N. We note that if N shrinks to P , then we have the expected time to "reach" P, conditioned on initial position. We also note that $T(x) \equiv 0$ if $x \in N$.

We seek a solution of (3.9) in the form

$$\begin{aligned} T(x) &= g(x)Q(\psi/\varepsilon^{1/4}, \alpha/\varepsilon^{1/2}, \beta/\varepsilon^{3/4}, 1/\varepsilon^{1/2}, \gamma_1/\varepsilon^{1/4}, \gamma_2) \\ &\quad + h(x)\varepsilon^{3/4}Q'(\psi/\varepsilon^{1/4}, \alpha/\varepsilon^{1/2}, \beta/\varepsilon^{3/4}, 1/\varepsilon^{1/2}, \gamma_{1/\varepsilon}{}^{1/4}, \psi_2) \qquad (4.25) \\ &\quad + k(x) \end{aligned}$$

where $Q(z,\alpha,\beta,\gamma_1,\gamma_2,\gamma_3)$ satisfies

$$\frac{d^2Q}{dz^2} = \pm\, (z^3 - \alpha z - \beta)\, \frac{dQ}{dz} - \gamma_1 + \gamma_2 z + \gamma_3 z^2 \qquad (4.26)$$

The (+) sign in (4.26) corresponds to the steady state P being stable, the (-) sign to it being unstable. We consider the case in which P is stable.

Instead of (4.5), we obtain

$$b^i\psi_i + \frac{a^{ij}}{2}\,\psi_i\psi_j\,(\psi^3 - \alpha\psi - \beta) = 0. \qquad (4.27)$$

When there are three steady states, α and β are determined by a procedure analogous to the one in section 4.2. Namely, at the steady states we set

$$\psi^3 - \alpha\psi - \beta = 0. \tag{4.28}$$

The method of characteristics is then used to determine α and β by an iterative procedure. When the three steady states coalesce $\alpha = \beta = 0$. When there is one real and two imaginary steady states, then $\alpha, \beta < 0$ and can be determined by power series. Such series are constructed elsewhere (10).

Instead of (4.7), we obtain

$$b^i k_i + \frac{a^{ij}}{2} \psi_i \psi_j g(-1+\gamma_2\psi+\gamma_3\psi^2) = -\bar{u}(x) \tag{4.29}$$

At the steady states, we obtain

$$\frac{a^{ij}}{2} \psi_i \psi_j g(-1+\gamma_2\psi+\gamma_3\psi^2) = -\bar{u}(x) \tag{4.30}$$

When there are three real steady states, we obtain three equations for g, γ_2, and γ_3. When two steady states coalesce, $\gamma_3 = 0$. We still have two equations for g and γ_2. Finally, when all three coalesce, $\gamma_2 = \gamma_3 = 0$ and we are left with one equation for g.

We obtain an equation for h(x) that is analogous to (4.13), and is treated in an analogous fashion. The initial values of Q and Q' in (4.26) are determined so that $T(x) \equiv 0$ if $x \in \partial N$.

4.4 HOPF CASE

The Hopf type dynamical system is treated in an identical fashion to the marginal and critical type systems. We seek a solution of (3.9) in the form

$$
\begin{aligned}
T(x) = {} & g(x)H(\psi/\varepsilon^{1/4}, \beta/\varepsilon^{1/2}, 1/\varepsilon^{1/2}, \gamma_2/\varepsilon^{1/4}) \\
& + {}^{1/4}H'(\psi/\varepsilon^{1/4}, 1/\varepsilon^{1/2}, \beta/\varepsilon^{1/2}, \gamma_2/\varepsilon^{1/4})h(x) \qquad (4.31) \\
& + k(x)
\end{aligned}
$$

where $H(z,\beta,\gamma_1,\gamma_2)$ satisfies

$$\frac{d^2H}{dt^2} = \pm (z^3 - \beta z) \frac{dH}{dz} - \gamma_1 + \gamma_2 z \qquad (4.32)$$

The (+) sign corresponds to a stable limit cycle and unstable focus, the (-) sign corresponds to an unstable limit cycle and stable focus. The analysis proceeds exactly as in section 4.2,3.

SECTION 5

SUBSTRATE INHIBITED REACTIONS: A MARGINAL TYPE STEADY STATE

The following equations model a substrate inhibited chemical reaction in an open reactor (10,14):

$$\dot{x}^1 = \frac{-1.4x^1}{1.5+x^1+13(x^1)^2} - .069979\, x^1 + .25901 - \frac{-x^1x^2}{1+10x^1x^2} \tag{5.1}$$

$$\dot{x}^2 = .09 - \frac{x^1x^2}{1+10x^1x^2}\ , \tag{5.2}$$

where x^1 and x^2 are dimensionless "concentration" variables. The steady state (.4359, 2.065) is a saddle node, it is a marginal type steady state. The steady state (1.46, .52) is a stable node. The phase portrait is shown in figure 8, along with a first exit boundary. The theory on section 4.2 applies. We wish to calculate the expected time to hit R, conditioned on initial position. Using the birth and death approach to chemical kinetics (15), εa can be modeled as (10):

$$\varepsilon a = \begin{pmatrix} (\lambda_1+\mu_1)x^1 & \dfrac{x^1x^2}{1+10x^1x^2} \\ \dfrac{x^1x^2}{1+10x^1x^2} & (\lambda_2+\mu_2)x^2 \end{pmatrix} \tag{5.3}$$

where

$$(\lambda_1+\mu_1)x^1 = \frac{1.4x^1}{1.5+x^1+13(x^1)^2} + .069979x^1 + .25901 + \frac{x^1x^2}{1+10x^1x^2} \tag{5.4}$$

$$(\lambda_2\mu_2)x^2 = .09 + \frac{x^1x^2}{1+10x^1x^2} \tag{5.5}$$

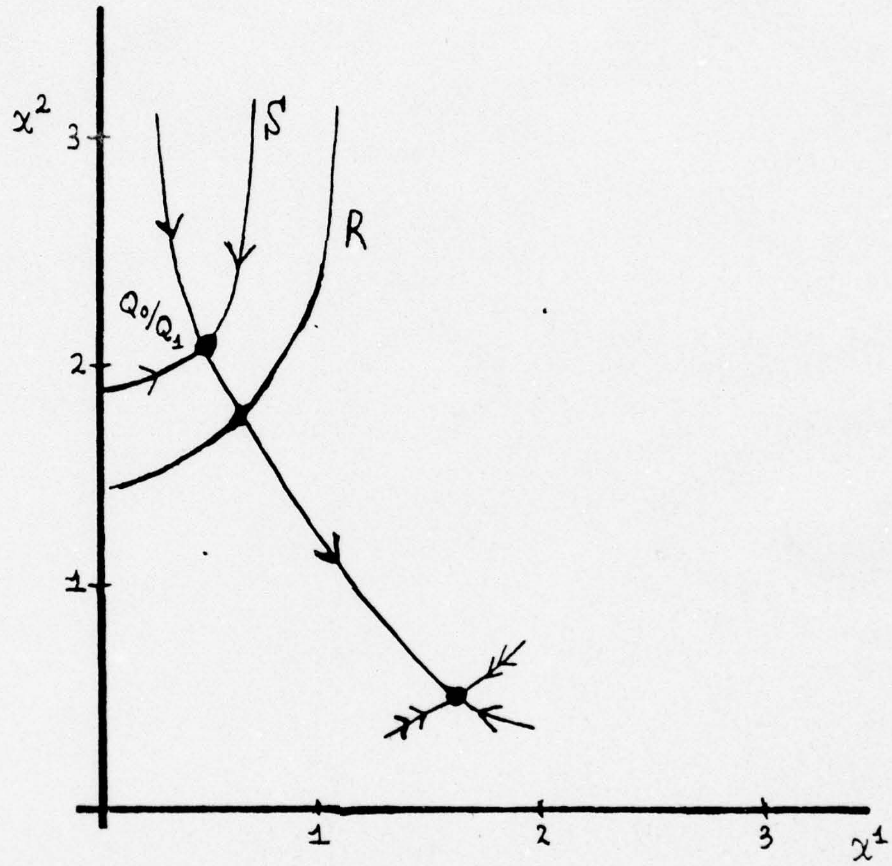


FIGURE 8: DETERMINISTIC PHASE PORTRAIT AT THE MARGINAL BIFURCATION. THE BOUNDARY R WAS USED IN THE CALCULATION OF THE MEAN EXIT TIME.

The parameter ε characterizes the intensity of fluctuation.

In table I, we compare the theory of section 4 with Monte Carlo experiments for $\varepsilon = .01$.

TABLE 1

Comparison of the Theory and Monte Carlo Experiments

in the Marginal Bifurcation

Test Point	T(x) Theory	T(x) Experiment (# Trials)
(.42, 2.06)	60.3	56.4 (950)
(.38, 2.36)	104.1	91.2 (400)
(.20, 2.0)	66.1	62.4 (2000)
(.3, 1.8)	37.7	35.0 (1550)
(.16, 2.4)	119.6	103.5 (400)
(.7, 2.2)	36.1	31.4 (1750)
(.6, 2.4)	74.9	68.2 (800)

SECTION 6

KINETIC MODEL OF THE FERROMAGNET

We shall give an analysis of the mean field ferromagnet, similar to that of Griffiths et. al. (2). The problem is one dimensional, so that the full theory of section 4 is not needed. However, this application illustrates many of the ideas that run through an analysis.

Consider N spins, with $\sigma_i = \pm 1$, in a magnetic field H. Let J be a coupling constant. The Hamiltoman is

$$\tilde{H} = \frac{-J}{N} \sum_{1<n} \sigma_i \sigma_j - \mu H \sum \sigma_i - 1/2J \tag{6.1}$$

We let

$$n = \frac{1}{2} (N + \Sigma\sigma_i) \ , \tag{6.2}$$

denote the number of spins "pointing up." Then (6.1) becomes

$$\tilde{H} \equiv \Phi(n) = \frac{-J(2n - N)^2}{2N} - \mu H(2n - N) \tag{6.3}$$

We take a mean field approach and assume that the number of spins pointing up is really a statistical variable, $\tilde{n}(t)$. The statistical behavior of $\tilde{n}(t)$ is described by transition probabilities:

$$\Pr\left\{\tilde{n}(\tau + \delta\tau) - \tilde{n}(\tau) = 1 \middle| \tilde{n}(\tau) = n\right\} \tag{6.4}$$

$$= \frac{N - n}{N} \exp\left[\frac{-\beta}{2}\left(\Phi(n + 1) - \Phi(n)\right)\right] \delta\tau + o(\delta\tau)$$

$$\Pr\left\{\tilde{n}(\tau+\delta\tau)-\tilde{n}(\tau) = -1 \,|\, \tilde{n}(\tau) = n\right\} \tag{6.5}$$

$$= \frac{n}{N}\exp\left[\frac{-\beta}{2}\left(\Phi(n-1)-\Phi(n)\right)\right]\delta\tau + o(\delta\tau) \;,$$

where $\beta = 1/k_B T$. We assume that the probability of all other transitions is $o(\delta\tau)$. In deriving (6.4,5), we have restated the argument in (2). We follow (2) and introduce a "continuous" variable

$$\tilde{x}(t) = \frac{\Sigma\sigma_i}{N} = \frac{2\tilde{n} - N}{N} \tag{6.6}$$

If $\delta\tilde{x} = \tilde{x}(\tau+\delta\tau) - \tilde{x}(\tau)$, then (6.4,5) become

$$\Pr\left\{\delta\tilde{x} = 2/N \,\middle|\, \tilde{x}(\tau) = x\right\} = \frac{1-x}{2}\exp\left\{-\beta\left(-xJ - \frac{J}{N} - H\mu\right)\right\}\delta\tau + o(\delta\tau) \tag{6.7}$$

$$\Pr\left\{\delta\tilde{x} = -2/N \,\middle|\, \tilde{x}(\tau) = x\right\} = \frac{1+x}{2}\exp\left\{-\beta\left(xJ - \frac{J}{N} + H\mu\right)\right\}\delta\tau + o(\delta\tau) \tag{6.8}$$

We set $\alpha = J\beta$, $\delta = \beta\mu H$ and introduce a macroscopic "physical" time defined by

$$t \equiv \frac{\tau}{N} \tag{6.9}$$

Thus, we construct drift and diffusion coefficients

$$b(x) = \lim_{\delta t\to 0}\frac{1}{\delta t}E\left\{\delta\tilde{x} \,|\, \tilde{x}(t) = x\right\} \tag{6.10}$$

$$= (1-x)\exp\left[\alpha x + \frac{\alpha}{N} + \delta\right] - (1+x)\exp\left[-\alpha x + \frac{\alpha}{N} - \delta\right] \tag{6.11}$$

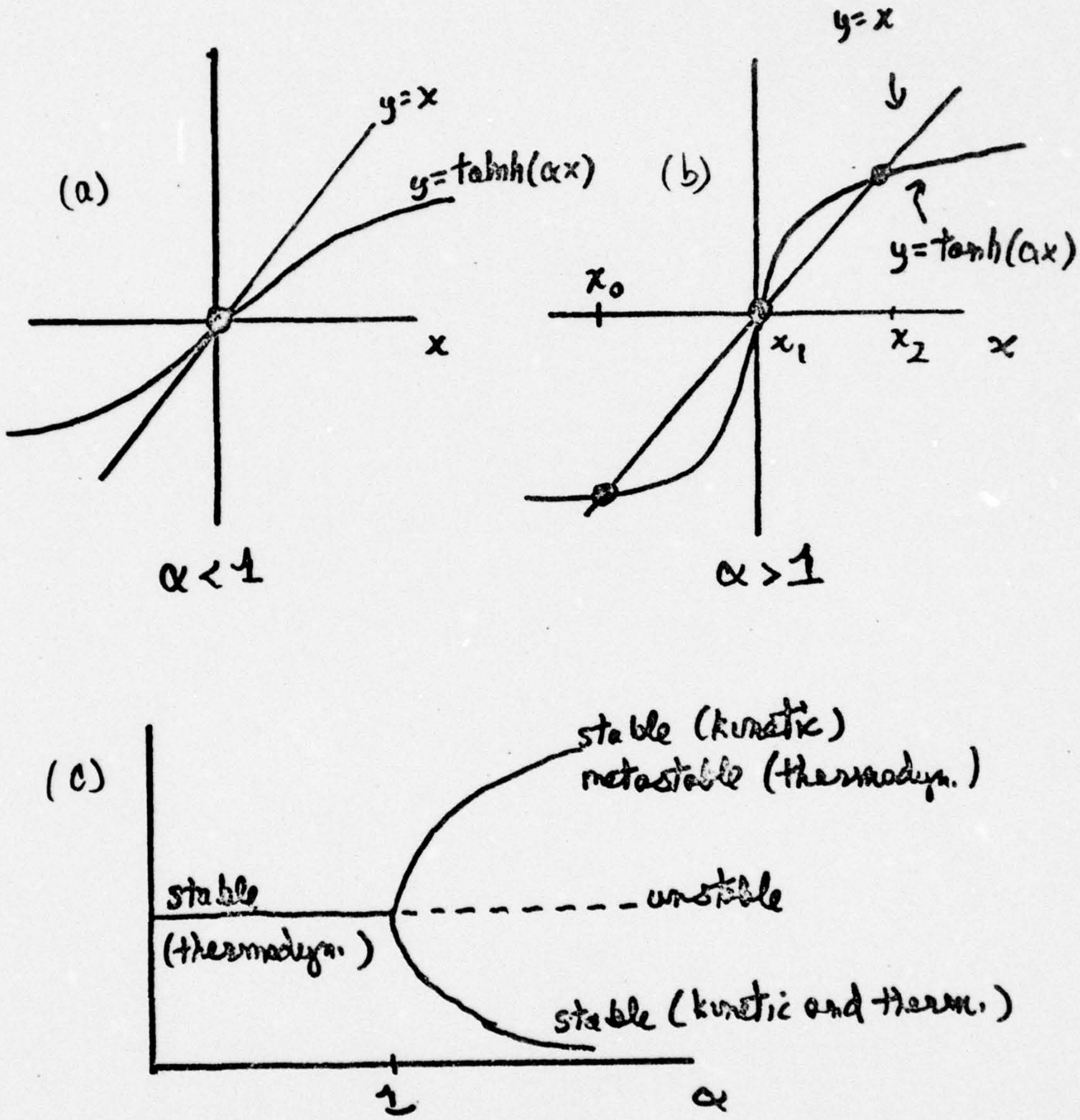


FIGURE 9: MEAN FIELD FERROMAGNET

and

$$a(x) = \lim_{\delta t \to 0} \frac{1}{\delta t} E \left\{ (\delta \tilde{x})^2 | \tilde{x}(t) = x \right\} \tag{6.12}$$

$$= \frac{1}{N} \left\{ (1 - x) \exp \left(\alpha x + \frac{\alpha}{N} + \delta\right) + (1 + x) \exp\left(-\alpha x + \frac{\alpha}{N} - \delta\right) \right\} \tag{6.13}$$

Thus, the average value of $\tilde{x}(t)$ evolves according to

$$\dot{x} = b(x,\alpha,\delta) = 2e^{\alpha/N} \left\{ \sinh(\alpha x + \delta) - x \cosh(\alpha x + \delta) \right\} , \tag{6.14}$$

subject to $-1 \leq x \leq 1$. The steady states and true (physical) equilibrium are solutions of $b(x,\alpha,\delta) = 0$. Therefore, one obtains

$$x = \tanh(\alpha x + \delta) \tag{6.15}$$

Equation (6.15) is usually obtained by a statistical thermodynamics argument (e.g. (16), pg. 101).

This agreement adds support to our statistical approach. In many respects, the approach used here is preferable to the standard approach. Not only does the stochastic approach yield the equilibrium solution, it gives dynamics and the steady states. As is well known, equation (6.15) may have 1, 2, or 3 solutions, depending upon the values of α and δ. In figures 9a, b, we illustrate the graphical solution of (6.15) for zero field ($\delta = 0$). When $\delta = 0$, x_0 and x_2 are both thermodynamically, and kinetically, stable. However, for $\delta \neq 0$, one of x_0, x_2 becomes kinetically stable (thermodynamically metastable) while the other is the true thermodynamic (and kinetic) equilibrium (Figure 9c). The kinetic condition of criticality is that, when $\delta = 0$

$$b'(x_1) = b''(x_1) = 0 \tag{6.16}$$

We easily obtain $\alpha = 1$ as the critical value of α. This defines the critical temperature.

Now consider $\delta \neq 0$, with x_0 metastable and x_2 stable. The expected time to reach x_2, given that $\tilde{x}(0) = x$ satisfies

$$-1 = \frac{a}{2}T_{xx} + bT_x \tag{6.17}$$

$$T(x_2) = 0 \qquad \lim_{x \to -\infty} T(x) < \infty \tag{6.18}$$

with $a(x)$ and $b(x)$ given by (6.13) and (6.11). Define the relaxation rate from the metastable to stable state by

$$k = \frac{1}{T(x_0)} \; . \tag{6.19}$$

We can calculate the relaxation rate k for all values of N. The method of Griffiths et.al. (2) broke down for large N. The result given here will be valid for all values of N. Our result thus extends their analysis. It can be shown that the two results are equivalent for small N.

SECTION 7

RELAXATION OF A CRITICAL HARMONIC OSCILLATOR

The application in section 6 did not use the theory of section 4, but the one in this section does. We consider a Duffing oscillator

$$\frac{dx}{dt} = v \tag{7.1}$$

$$\frac{md\,v}{dt} = (-k(\eta)x - \alpha(x^3) - \gamma v) + \sqrt{\varepsilon a}\,\frac{d\tilde{y}}{dt} \tag{7.2}$$

We assume that $k(\eta c) = 0$ for some critical value of η and that $k(\eta) \geq 0$ for all η. The mean motion of the oscillator is given by

$$\dot{x} = v \tag{7.3}$$

$$\dot{v} = \frac{-kx-\alpha x^3-\gamma v}{n} \tag{7.4}$$

When $\alpha > 0$, the origin is the only real steady state. The matrix

$$B = (b^i{}_{,j})\big|_{0,0} = \begin{pmatrix} 0 & 1 \\ \frac{-k}{m} & \frac{-\gamma}{m} \end{pmatrix} \tag{7.5}$$

has eigenvalues and eigenvectors

$$\lambda_{\pm} = \frac{-\gamma \pm \sqrt{\gamma^2-4k}}{2m} \qquad e_{\pm} = \begin{pmatrix} 1 \\ \frac{-\gamma \pm \sqrt{\gamma^2-4k}}{2m} \end{pmatrix} \tag{7.6}$$

when $k \equiv 0$, the origin is a critical type steady state. According to the fluctuation dissipation theorem, for this problem $a = 2kT\gamma\rho$, where

$$\rho = \int_0^\infty E(\tilde{y}(s)\tilde{y}(0))ds \tag{7.7}$$

Let $T(x,v)$ be the expected time that the process takes to enter a small ellipse around the origin, given that $\tilde{x}(0) = x$, $\tilde{v}(0) = v$. Then, for arbitrary k ,

$$-1 = \frac{kT\gamma\rho}{m^2} T_{vv} + vT_x - \frac{(kx+\alpha x^3+\gamma v)}{m} T_v \tag{7.8}$$

We introduce scaled variables by

$$\left.\begin{array}{lll} v = \sqrt{\dfrac{E_0}{m}}\, v' & T = \dfrac{m}{\gamma_0} T' & t = \dfrac{m}{\gamma_0} t' \\ x = \sqrt{\dfrac{E_0 m}{\gamma_0^2}}\, x' & \gamma = \gamma_0 \eta(x') & k = \dfrac{k'\gamma_0}{\sqrt{E_0 m}} \end{array}\right\} \tag{7.9}$$

$$\alpha = \gamma_0 \left(\frac{\gamma_0^2}{E_0 m}\right)^{3/2} \alpha'$$

Where E_0 is some reference energy, such that $\rho kT \ll E_0$. Defining $\epsilon = \rho kT/E_0$, we obtain (for $k(\eta) \equiv 0$)

$$-1 = \epsilon\eta T'_{v'v'} + v'T'_{x'} - (\alpha'(x')^3 + \eta' v')T'_{v'} \tag{7.10}$$

In the sequel, we drop the primes. Since the origin is a critical type steady state, the theory of section 4 applies.

The leading term in the asymptotic solution of (7.10) is

$$T(x) \sim g^0\, Q(\psi(x,v)/\epsilon^{1/4}, 0, 0, {}^1/\epsilon^{1/2}, 0, 0) \tag{7.11}$$
$$+k^0(x) + 0(\epsilon^{3/4})$$

Equations (4.27) and (4.29) become

$$v\psi_x - (\alpha x^3 + \eta v)\psi_v + \eta\psi_v^2\psi^3 = 0 \tag{7.12}$$

$$vk_x^0 - (\alpha x^3 + \eta v)k_v^0 - g^0 \frac{\eta}{2}\psi_v^2 = -1 \tag{7.13}$$

In order to keep ψ regular at (0,0), we set $\psi = 0$ there. In order to solve (7.12) by the method of characteristics, we need initial data for ψ_x and ψ_v. If (7.12) is differentiated with respect to v and evaluated at (0,0), we obtain

$$\psi_x - \eta\psi_v = 0 \quad \text{at } (0,0) \tag{7.14}$$

When (7.12) is differentiated three times with respect to x and evaluated at (0,0), we obtain

$$\psi_x^3\psi_v^2 = \alpha/\eta \tag{7.15}$$

Thus we obtain, at (0,0)

$$\psi_x = (\alpha\eta)^{1/5} \qquad \psi_v = \left(\alpha^{1/5}\right)\cdot\left(\eta^{4/5}\right)^{-1} \tag{7.16}$$

Higher derivatives are evaluated in a similar fashion. Thus, we can specify an ellipse around the origin:

$$N = \left\{(x,v) : \psi(x,v) = \delta\right\} \tag{7.17}$$

We set $Q(\delta/\varepsilon^{1/4},0,0,1/\varepsilon^{1/2},0,0) = Q'(\delta/\varepsilon^{1/4},0,0,1/\varepsilon^{1/2},0,0) = 0$ when integrating (4.26). We also set $k(x,v) = 0$ if $(x,v) \in N$.

At the origin, (7.13) becomes

$$g^0 = \frac{2}{\eta\psi_v^2} = \frac{2}{\alpha^{2/5}}\eta^{3/5}, \tag{7.18}$$

which determines the value of g^0. Then, on deterministic trajectories we have

$$\frac{dk^0}{dt} = -1 + \frac{g^0 \eta \psi_v^2}{2} \tag{7.19}$$

with the initial data given above. Equation (7.12) can now be solved by the method of characteristics, so that the leading term in the asymptotic solution is known.

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Appendix: Classification of Two Dimensional Dynamical Systems. The Normal Forms for Marginal and Critical Type Deterministic Systems

In this appendix, we classify planar dynamical systems into normal, marginal, or critical types. Our scheme is a generalization of the work of Kubo et.al. (4). We use Segre's method (17) to derive the local normal forms for the marginal and critical cases.

I. Normal Type Dynamical Systems

Let the dynamical system

$$\dot{x} = b(x) \qquad x \in R^2 \tag{A.1}$$

have a steady state at $x = x_0$. Let $\lambda\pm$ denote the eigenvalues of $(b^i_{,j})$ evaluated at x_0. The system (A.1) is of the normal type if the real parts of $\lambda\pm$ are non-zero. The steady state is stable if the real parts of $\lambda\pm$ are negative.

According to the standard theory of differential equations (18) there exists a change of variables $x \to y$ so that

$$\begin{pmatrix} \dot{y}_1 \\ \dot{y}_2 \end{pmatrix} = \begin{pmatrix} \lambda+ & 0 \\ 0 & \lambda- \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} + \begin{pmatrix} ay_1^2 + b\, y_1 y_2 + cy_2^2 \\ a_2 y_2^2 + b_2 y_1 y_2 + c_2 y_2^2 \end{pmatrix} + 0(y^3)$$

The coefficients $a_i - c_i$ are given in terms of the second derivatives of $b(x)$ evaluated at x_0.

II. The Marginal Type Systems

The dynamical system

$$\dot{x} = b(x,\eta) \qquad x \in R^2 \quad \eta \in R \tag{A.2}$$

is assumed to have the following behavior. (A.2) is assumed to have three real steady states for $\eta > 0$. We denote these by $Q_0(\eta)$, $Q_1(\eta)$ P_2.

Denote by B_k the matrix $(b^i_{,j})$ evaluated at Q_0, Q, or P_2. $(k=0,1,2)$.

We assume

1) For all η, B_2 has two real negative eigenvalues

2) As $\eta \downarrow 0$, the distance between $Q_0(\eta)$ and $Q_1(\eta)$ decreases. When $\eta = 0$ the two points coalesce and annihilate each other

3) For $\eta > 0, B_0$ has two real, negative eigenvalues which depend upon η and B_1, has one real positive and one real negative eigenvalue. When $\eta = 0$, $B_0 = B_1$ has one zero and real negative eigenvalue. The eigenvector corresponding to the negative eigenvalue has positive slope.

We introduce as new coordinates the eigenvectors y_1, y_2 as new coordinates so that (A.2) becomes

$$\dot{y}_1 = \tilde{b}^1(y,\eta)$$
$$\dot{y}_2 = \tilde{b}^2(y,\eta) \tag{A.2a}$$

The system (A.2) is of the marginal type if the above conditions hold and

a) $$\frac{\partial \tilde{b}^1}{\partial y_1}(0,0) = 0 \tag{A.3}$$

b) $$\frac{\partial^2 \tilde{b}^1}{\partial y_1^2}(0,0) \equiv a \neq 0.$$

When η is small, but non-zero, we translate the origin, so that the system (A.2) is approximately given by

$$\begin{cases} \dot{y}_1 = \tilde{c}_1\eta + \tilde{c}_2\eta y_1 + ay_1^2 + \tilde{b}y_1y_2 + \tilde{c}y_2^2 \\ \qquad\qquad + 0\,(y^3,\eta^2) \\ \dot{y}_2 = \tilde{\lambda}(\eta)y_2 + 0(y^2,\eta) \end{cases} \tag{A.4}$$

In (A.4), $\tilde{\lambda}(\eta)$ is the non-zero eigenvalue of $B(\eta) = (b^i_{,j}(\eta))|x_1$. The coefficient a is given by A.3b; the other coefficients are also given in terms of the derivatives of $b(x)$. We assume $c_1 \mp 0$

Let $y' = \frac{1}{a}\dot{y}$. Then (A.4) becomes

$$\left.\begin{aligned} y_1 &= c_1\eta + c_2\eta y_1 + y_1^2 + by_1y_2 + cy_2^2 + 0(y^3,\eta^2) \\ y_2' &= \lambda_0 y_2 + 0(y^2,\eta) \end{aligned}\right\} \tag{A.5}$$

where $s = \tilde{s}/a$.

Introduce new coordinates by

$$\left.\begin{aligned} z_1 &= y_1+sy_1y_2+ty_1^2+uy_2^2+wy_1\eta+ry_2\eta \\ &\qquad + 0\,(\eta^2,y^3,\eta y^2) \\ z_2 &= y_2 + 0(\eta,y^2) \end{aligned}\right\} \tag{A.6}$$

then

$$
\left.\begin{aligned}
Z_2' &= Y_2' = \lambda_0 Z_2 + 0(\eta, Z^2) \\
Z_1' &= Y_1' + sY_1'Y_2 + sY_1Y_2' + 2tY_1Y_1' \\
&\qquad +2uY_2Y_2' + wY_1'\eta + rY_2'\eta \\
&\qquad + 0(\eta YY', Y^2Y')
\end{aligned}\right\} \tag{A.7}
$$

Using (A.5) in (A.7) yields

$$
\left.\begin{aligned}
Z_2' &= \lambda_0 Z_2 + 0(\eta, Z^2) \\
Z_1' &= c_1\eta + Y_1(c_2\eta + 2tc_1\eta) + Y_1^2 \\
&\quad + Y_1Y_2(b + s\lambda_0) + Y_2(r\eta\lambda + sc_1\eta) \\
&\quad + Y_2^2(2u\lambda + c) + 0(Y^3, \eta Y^2 . \eta^2)
\end{aligned}\right\} \tag{A.8}
$$

We choose

$$
t = \frac{-c_2}{2c_1} \qquad 5 = \frac{-b}{\lambda_0} \qquad r = \frac{-sc_1}{\lambda}
$$

$$
u = \frac{-c}{2\lambda}
$$

and note that $Y_1^2 = Z_1^2 + 0(Y^3)$. Thus equation (A.8) becomes

$$
\begin{aligned}
Z_2' &= \lambda_0 Z_2 + 0\ (\eta, Z^2) \\
Z_1' &= Z_1^2 - \beta(\eta) + 0(Z^3, \eta Z^2, \eta^2)
\end{aligned} \tag{A.9}
$$

where $\beta(\eta) = -c_1\eta$. Equation (A.9) is the local normal form which we desire. It is a weaker result than that of Arnol'd (5) or Shoshaitshvili (6) who actually eliminate the higher order terms.

III. Critical Type Systems

We now consider a dynamical system depending upon two parameters

$$\dot{x} = b(x,\eta,\delta) \qquad x\in R^2 \qquad \eta,\delta\in R \tag{A.10}$$

We make the following assumptions:

1) For some combinations of η and δ, equation (A.10) has three steady states $P_0(\eta,\delta)$, $P_1(\eta,\delta)$ and $P_2(\eta,\delta)$. When the three points are distinct, we assume that P_0 and P_2 are stable nodes and that P_1 is a saddle point.

2) As η,δ vary, two of the points may coalesce into a point of neutral stability (i.e., one eigenvalue of the linearized equations is zero). This situation is equivalent to a marginal type dynamical system.

3) As $\eta,\delta \to 0$ from above, the three steady states approach each other and coalesce when $\eta = \delta = 0$. Let $B = (b^i_{,j})$ evaluated at P_1. When $\eta,\delta>0$, we assume that B has one real positive and one real negative eigenvalue. When $\eta = \delta = 0$, B has one real negative and one zero eigenvalue. When $\eta,\delta<0$, B has two real negative eigenvalues.

We denote by $y_1(\eta,\delta)$, $y_2(\eta,\delta)$ the eigenvectors of B.

The eigenvectors y_1, y_2 are introduced as new coordinates so that (A.10) becomes

$$\dot{y}_1 = \tilde{B}^1(y,\eta,\delta)$$
$$\dot{y}_2 = \tilde{B}^2(y,\eta,\delta) \tag{A.10a}$$

The system A.10a is of the critical type if

a) at $\eta = \delta = 0$, B has one zero eigenvalue

b) the second derivatives

$$\left.\frac{\partial^2 \tilde{B}}{\partial y_1^2}\right|_{(0,0,)} , \quad \frac{\partial^2 \tilde{B}}{\partial y_1 \partial y_2} , \quad \frac{\partial^2 \tilde{B}}{\partial y_2^2} \quad \text{vanish} \tag{A.11}$$

when $\eta = \delta = 0$

c) $$\frac{\partial^2 \tilde{B}}{\partial y_1^3} = a \neq 0 .$$

The assumption on A.10b can actually be weakened slightly: we only need to require that $\frac{\partial^2 \tilde{B}}{\partial y_1^2}$ vanish, the other second derivatives need not vanish. However, assumption A.10b does not cause any loss of generality and simplifies the analysis considerably.

In terms of the y coordinates, for small η,δ the system (A.10) takes the form

$$\dot{y}_2 = \tilde{\lambda}(\eta,\delta)y_2 + 0(y^2,(\eta + \delta)y)$$

$$\dot{y}_1 = \tilde{c}_1\eta + \tilde{c}_2\delta + y_1(\tilde{c}_3\eta + \tilde{c}_4\delta) \tag{A.12}$$
$$+ y_1^2(\tilde{c}_5\eta + \tilde{c}_6\delta) + y_1y_2(\tilde{c}_7\eta + c_8\tilde{\delta})$$

$$+ y_2^2(\tilde{c}_9\eta + \tilde{c}_{10}\delta) + ay_1^3 + \tilde{b}y_1^2y_2$$

$$+ \tilde{c}y_1y_2^2 + \tilde{d}y_2^3 + 0(y^4, (\eta^2 + \delta^2)y_1 \qquad \text{(A.12) cont'd}$$

$$(\eta + \delta)y^3)$$

Letting $y' = \frac{1}{a}\dot{y}$, $s = \tilde{s}/a$ and $\delta_i = c_{2i-1}\eta + c_{2i}\delta$ we have

$$y_2' = \lambda_0 y_2 + 0(y^2, (\eta + \delta)y)$$

$$y_2' = \gamma_1 + \gamma_2 y_1 + \gamma_3 y_1^2 + \gamma_4 y_. y_2 \qquad \text{(A.13)}$$

$$+ \gamma_5 y_2^2 + y_1^3 + by_1^2 y_2$$

$$+ cy_1y_2^2 + dy_2^3$$

$$+ 0(y^4, (\eta^2 + \delta^2)y,$$

$$(\eta + \delta)y^3)$$

We now introduce new variables by

$$z_2 = y_2 + 0(y^2, (\eta + \delta)y)$$

$$z_1 = y_1 + s_1\eta y_1^2 + t_1\eta y_1 y_2 + u_1\eta y_2^2$$

$$+ s_2\delta y_1^2 + t_2\delta y_1 y_2 + u_2\delta y_2^2 \qquad \text{(A.14)}$$

$$+ w_1y_1^3 + w_2y_1^2y_2 + w_3y_1y_2^2$$

$$+ w_4y_2^3 + 0(y^4, (\eta^2 + \delta^2)y, \eta y^3)$$

Without loss of generality, we have not included terms $0(y^2)$ in the definition of z_1. This follows from assumption A.10b.

From A.14, we have

$$Z_2 = y_2 + 0(yy\ ,(\eta + \delta)y\ )$$

$$Z_1' = y_1' + 2s_1\eta y_1 y_1' + t_1\eta y_1 y_2' \qquad (A.15)$$

$$+ t_1\eta y_1' y_2 + 2u_1\eta y_2 y_2 + 2 s_2 y_k y_k' \delta$$

$$+ t_2\delta(y_1 y_2' + y_1' y_2) + 2u_2\delta y_2 y_2'$$

$$+ 3w_1 y_1^2 y_1' + w_2(y_1' y_1 y_2 + y_1^2 y_2')$$

$$+ w_3(y_1' y_2^2 + 2y_1 y_2 y_2')$$

$$+ 3w_4 y_2^2 y_2'$$

$$+ 0(y^3 y', \eta^2 y', \delta^2 y')$$

Using (A.13) in (A.15) yields (with $\lambda = \lambda_0$)

$$Z_2' = \lambda_0 Z_2 + 0(Z^2, \eta Z)$$

$$Z_1' = \gamma_1 + y_1\ \gamma_2$$

$$+ y_1^2(\gamma_3 + 3w_1\gamma_1)$$

$$+ y_1 y_2(\gamma_4 + t_1\eta\lambda + t_2\delta\lambda + w_2\lambda_1 + 2\lambda w_3) \qquad (A.16)$$

$$+ y_2^2(\gamma_5 + 2u_1\eta\lambda + 2u_2\delta\lambda + w_3\lambda_1)$$

$$+ y_1^3$$

$$+ y_1^2(b + w_2\lambda + w_2\lambda + w_2\gamma_2)$$

$$+ y_1 y_2^2 (c + 2w_3\lambda + w_3 \ \gamma_2)$$

$$+ y_2^3 (d + 3w_4\lambda)$$

$$+ 0(y^4, (\eta^2 + \delta^2)y, y^3(\eta + \delta)$$

We choose

$$w_4 = \frac{-d}{3\lambda} \qquad w_3 = \frac{-c}{2\lambda+\gamma_2} \qquad w_2 = \frac{-b}{\lambda+\gamma_2}$$

$$u_1\eta + u_2\delta = \frac{-\gamma_5 - w_3\gamma_1}{2\lambda}$$

$$t_1\eta + t_2\delta = \frac{-\gamma_4 - w_2\gamma_1 - 2\lambda w_3}{\lambda}$$

$$w_1 = \frac{-\gamma_3}{3\gamma_1} \quad .$$

Noting that $y_1^3 = z_1^3 + 0(\eta y^3, \eta^2 y^2)$ and

that $y_1\gamma_1 = z_1\gamma_1 + 0(\eta^2 z^2)$, egn (A.16)

becomes

$$z_2' = \lambda_0 z_2 + 0(z^2, \eta z)$$

$$z_1' = \gamma_1 + \gamma_2 z_1 + z_1^3 + 0(z^4, (\eta^2 + \delta^2),$$

$$(\eta + \delta)z^3),$$

which is the desired normal form.

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